

MCULE PROTECTED BUILDING BLOCK LIBRARY

MCULE PROTECTED BUILDING BLOCK LIBRARY MEMBERS CONTAIN AT LEAST ONE COMMONLY APPLIED PROTECTING GROUP FOR SELECTIVE SYNTHESIS AND COMPLEX REACTIONS.

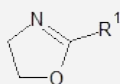
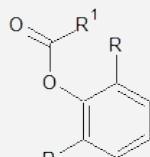
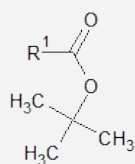
Protecting chemical groups were defined as SMARTS patterns and a comprehensive search was carried out on the full Mcule database to identify all building blocks with at least one match. The identified molecules may contain more than a single protecting group enabling multi-step synthesis using masked sensitive functional groups, such as amines, carboxylic acids, alcohols or carbonyls.

Please find below the full list of the included protecting groups.

Protected building blocks are compounds with specific chemical functionalities temporarily protected by chemical groups. The application of protected building blocks is a useful strategy in organic synthesis to enable chemists to carry out complex, precise and selective reactions, protect sensitive functional groups, and expedite the synthesis of new compounds.

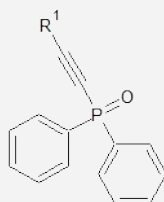
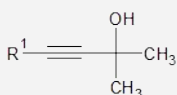
Carboxyls:

- Methyl ester
- t-Butyl ester
- Benzyl ester
- S-t-Butyl ester
- 2,6-disubstituted phenyl esters
- Silyl esters
- Oxazoline

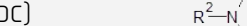


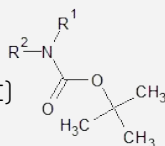
Terminal alkynes:

- Propargyl R^1
- Silyl
- Diphenylphosphoryl

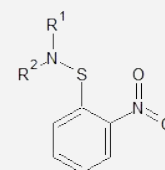
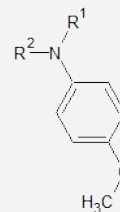
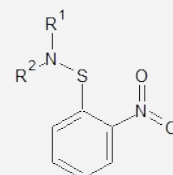


Amines:


- t-Butyl carbamate (Boc)
 - 9-Fluorenylmethyl carbamate (Fmoc)
 - Triphenylmethylamine (Trityl)
 - Benzyl carbamate (Cbz)
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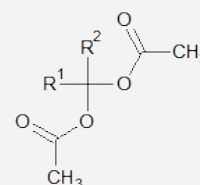
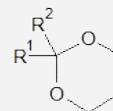


- Phthalimide
- p-toluene-sulfonamide
- Benzylideneamine
- Trifluoroacetamide
- t-Butanoic amide
- Benzoic amide R^2-N
- p-Methoxy-phenyl \langle
- p-Methoxy-benzyl
- 3,4-Dimethoxy-benzyl
- Trichloroethyl-chloroformate
- p-methoxybenzyl-carbonyl
- Nosyl
- Nps



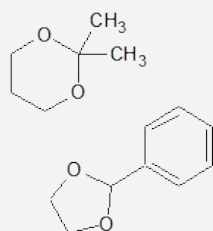
Carbonyls:

- 1,3-Dithiane
 - 1,3-Dioxane
 - Dimethyl acetal
 - N,N-Dimethylhydrazone
 - Acylal
- 



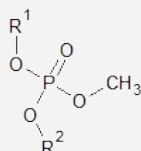
Diols:

- 1,3-Diol acetonide
- 1,3-Diol benzylidene acetal
- 1,2-Diol acetonide
- 1,2-Diol benzylidene acetal



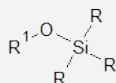
Phosphates:

- Methyl
- 2-Cyanoethyl

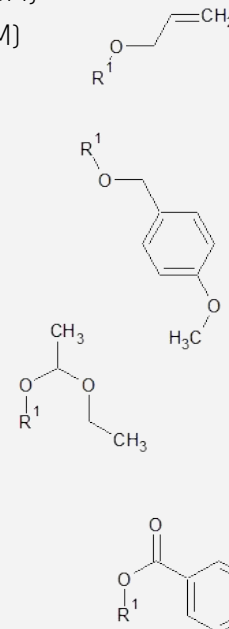


Hydroxyl:

- t-Butyl ether
- Silyl ethers (e.g. TBDMS, TBDPS,)



- Methoxymethyl ether (MOM)
- Ethoxymethyl ether (MEM)
- Allyl ether
- Benzyl ether
- Tetrahydropyranyl ether
- Tetrahydrofuranyl ether
- Methoxybenzyl
- Methoxyphenyl
- Trityl, dimethoxytrityl
- Methyl ether
- Ethoxyethyl ether
- Methylthiomethyl ether
- Acetic acid ester
- Pivalic acid ester
- Benzoic acid ester



Click [here](#) to access the downloadable data file of Mcule Protected Building Block Library. This CSV.GZ compressed file contains the SMILES structure of the compounds and separate columns for the number of occurrences of each functional group. The column names in the file indicate which chemical function is protected by which protecting group. For example, Carboxyl_PG_Oxazoline means the carboxyl group is protected by an oxazoline.

Mcule's complementary services to provide a complete compound sourcing solution

Professional laboratory services include:

- Transferring samples to plates/vials as solid or DMSO solution,
- Solubility characterization,
- Temperature controlled shipping,
- Quality control via LC-MS & NMR (on demand).

Please also reach out to our cheminformatics experts with projects related to

- Screening library building/expansion,
- Generation of synthetically feasible chemical spaces based on your building blocks,
- Filtering the Mcule database based on your criteria.

Mcule's Custom Solution Experts are ready to guide you through the selection and ordering process free of charge! If you have any questions or need any help, please feel free to contact us at support@mcule.com.